

The goal of this problem is to show that there are two equivalent expressions for the residual sum of squares in linear regression.

Let our training data be  $\{(x_1, y_1), \dots, (x_N, y_N)\}$ , where the vector  $x_n \in \mathbb{R}^D$  includes the  $D$  features and  $y_n \in \mathbb{R}$  is the label of sample  $n$ .

The training data can be also written in a matrix/vector notation as:

$$X = \begin{bmatrix} 1 & x_1^T \\ \vdots & \vdots \\ 1 & x_N^T \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1D} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \in \mathbb{R}^{N \times (D+1)} \text{ and } y = [y_1, \dots, y_N]^T \in \mathbb{R}^N$$

where  $x_{nd}$  is the  $d^{\text{th}}$  feature of sample  $n$ .

Let's also assume that the weight of the linear regression model is written as  $w = [w_0, w_1, \dots, w_D]$ , where  $w_0$  is the bias.

Show that the following expressions of the RSS error are equivalent:

$$RSS(w) = \sum_{n=1}^N \left[ y_n - \left( w_0 + \sum_{d=1}^D w_d x_{nd} \right) \right]^2$$

$$RSS(w) = (y - Xw)^T (y - Xw)$$

$$\begin{aligned} \vec{y} - X\vec{w} &= \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1D} \\ 1 & x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix} \\ &= \begin{bmatrix} y_1 - (w_0 + w_1 x_{11} + w_2 x_{12} + \dots + w_D x_{1D}) \\ \vdots \\ y_N - (w_0 + w_1 x_{N1} + w_2 x_{N2} + \dots + w_D x_{ND}) \end{bmatrix} \in \mathbb{R}^N \\ &\quad \text{the feature of each sample is multiplied by the corresponding weight.} \\ &\quad \sum_{d=1}^D w_d x_{nd} \\ \underbrace{(\vec{y} - X\vec{w})^T}_{\mathbb{R}^{1 \times N}} \underbrace{(y - X\vec{w})}_{\mathbb{R}^{N \times 1}} &= \begin{bmatrix} y_1 - (w_0 + \sum_{d=1}^D w_d x_{1d}), \dots, y_N - (w_0 + \sum_{d=1}^D w_d x_{Nd}) \end{bmatrix} \begin{bmatrix} y_1 - (w_0 + \sum_{d=1}^D w_d x_{1d}) \\ \vdots \\ y_N - (w_0 + \sum_{d=1}^D w_d x_{Nd}) \end{bmatrix} \\ &= \left( y_1 - \left( w_0 + \sum_{d=1}^D w_d x_{1d} \right) \right)^2 + \dots + \left( y_N - \left( w_0 + \sum_{d=1}^D w_d x_{Nd} \right) \right)^2 \\ &= \sum_{n=1}^N \left[ y_n - \left( w_0 + \sum_{d=1}^D w_d x_{nd} \right) \right]^2 \end{aligned}$$

Let  $\mathbf{x} = [x_1, x_2] \in \mathbb{R}^2$  be a 2-dimensional vector.

(1) Compute the first derivative and Hessian of the function  $f$ .

$$\frac{\partial f(\vec{x})}{\partial \vec{x}} = \begin{bmatrix} \frac{\partial f(\vec{x})}{\partial x_1} & \frac{\partial f(\vec{x})}{\partial x_2} \end{bmatrix}^T = \begin{bmatrix} 2(x_1 - 3x_2) & -6(x_1 - 3x_2) \end{bmatrix}^T \in \mathbb{R}^2$$

$$H_{f(\vec{x})} = \begin{bmatrix} \frac{\partial^2 f(\vec{x})}{\partial x_1^2} & \frac{\partial^2 f(\vec{x})}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f(\vec{x})}{\partial x_1 \partial x_2} & \frac{\partial^2 f(\vec{x})}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 2 & -6 \\ -6 & 18 \end{bmatrix} \in \mathbb{R}^{2 \times 2}$$

(2) Show that the function  $f(\mathbf{x}) = (x_1 - 3x_2)^2$  is convex by showing that its Hessian is positive semi-definite.

For any  $\vec{u} \in \mathbb{R}^2$ ,  $\vec{u} = [u_1, u_2]^T$ , we have:

$$\begin{aligned} \vec{u}^T H_{f(\vec{x})} \vec{u} &= [u_1 \ u_2]^T \begin{bmatrix} 2 & -6 \\ -6 & 18 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \\ &= [2u_1 - 6u_2, -6u_1 + 18u_2]^T \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \\ &= 2u_1^2 - 6u_1u_2 - 6u_1u_2 + 18u_2^2 \\ &= 2u_1^2 - 12u_1u_2 + 18u_2^2 \\ &= 2(u_1^2 - 6u_1u_2 + 9u_2^2) = 2(u_1 - 3u_2)^2 \geq 0 \end{aligned}$$

Therefore  $H_{f(\vec{x})}$   
positive semi-de  
so  $f(\vec{x})$  is convex

(3) Show that the function  $f(\mathbf{x}) = (x_1 - 3x_2)^2$  is convex by showing that the eigenvalues of its Hessian are non-negative.

$$\text{Det}(H_{f(\vec{x})}) = 0 \Rightarrow \begin{vmatrix} \lambda - 2 & -6 \\ -6 & \lambda - 18 \end{vmatrix} = 0 \Rightarrow \lambda^2 - 20\lambda + 36 - 36 = 0 \Rightarrow$$

$$\Rightarrow \lambda(\lambda - 20) = 0 \Rightarrow \lambda_1 = 0 \text{ and } \lambda_2 = 20$$

Both eigenvalues are non-negative, therefore  $H_{f(\vec{x})}$  is positive semi-definite, so  $f$  is convex.